

Pairing Correlations in the two-layer attractive Hubbard Model

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Studies of systems with two fermionic bands with *repulsive* interaction strength U have a long history, with the Periodic Anderson Model (PAM) being one of the most frequently considered Hamiltonians. In this paper, we use Quantum Monte Carlo to study analogous issues for *attractive* interactions. As in the Periodic Anderson Model, we focus on a case where one band is uncorrelated ($U = 0$), and focus on the effect of hybridization V between the bands on the pairing correlations. A key difference with the PAM is that there is no sign problem, so that we are able to explore the physics of *doped* multi-band attractive systems at low temperatures whereas ground state properties of repulsive models can be determined only at half-filling. For small V , pairing in the $U < 0$ layer induces pairing in the $U = 0$ layer. At larger V the ground state of the coupled system loses its superconducting character. The Quantum Monte Carlo data are complemented by results obtained with the Bogoliubov-de Gennes approximation.

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I. INTRODUCTION

Cuprate superconductors are characterized by CuO_2 planes which are rather isolated from each other by intervening rare earth atoms. The larger (“ c -axis”) separation of Cu atoms perpendicular to the planes compared to the in-plane lattice constants (a, b) has focused theoretical attention on the magnetic and superconducting properties of two-dimensional models, most notably the square lattice Heisenberg and Hubbard Hamiltonians. Indeed, one of the most fundamental theoretical questions which arose in the initial investigations of possible models of high temperature superconductivity concerned the nature of the magnetism in the ground states of these Hamiltonians: Were they spin-liquids or did they exhibit long range order? It was established numerically¹⁻³ that both the Heisenberg Hamiltonian and the half-filled Hubbard Hamiltonian have long range antiferromagnetic order at $T = 0$. A still-unresolved question is the nature of pairing in the doped Hubbard Hamiltonian.

A natural extension of these single layer questions concerns the behavior of spin and pairing correlations in coupled planes. Interlayer connections are required to elevate the magnetic ordering, which is possible only at $T = 0$ in two dimensions, to the finite temperature Néel transitions observed experimentally. Similarly, the superconducting transition temperature tends to increase with the number of adjacent CuO_2 layers between the charge reservoirs, getting steadily larger from single layered $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, to bilayer $\text{YBaCu}_3\text{O}_{6+y}$ to the HgBaCaCuO sequence where T_c peaks at about 130° K for materials with $n = 3$ layers⁴. Antiferromagnetism and thus superconductivity exhibit the expected behavior that

adding additional (non-frustrating) couplings, and increasing the dimensionality, enhances the tendency to order.

The route from 2D to 3D is, however, not completely straightforward. Quantum Monte Carlo (QMC) studies of coupled Heisenberg layers⁵, have shown that when the inter-plane coupling grows sufficiently large, there is a Quantum Phase Transition (QPT) from a ground state with long range magnetic order to a spin-gapped ground state, in which singlets form between pairs of spins in the two planes⁶. A similar effect is seen in QMC studies of the two-layer half-filled Hubbard Hamiltonian⁷.

The basic phenomenon of singlet formation usurping magnetic order in itinerant fermion Hamiltonians does not crucially depend on having the same interaction strength U , or hopping t , for the two species. Indeed, a Hamiltonian with $U = 0$ in one (conduction) band and hopping $t = 0$ in another (localized) band, is the commonly encountered Periodic Anderson Model (PAM). At half-filling, for weak hybridization between the conduction and localized bands, antiferromagnetic order is present. As the hybridization grows bigger, however, “Kondo” singlets form and destroy antiferromagnetic (AF) order. Thus the PAM exhibits a similar QPT as for two identical Hubbard layers ($t_1 = t_2$ and $U_1 = U_2$). This close similarity of the PAM and Hubbard bilayers emphasizes that the physics of fermions in multiple layers can equivalently be interpreted in terms of multiple orbitals.

The purpose of this paper is to study the possibility of analogous phenomena in the case when there is an *attractive* interaction. More specifically, we examine the nature of pairing correlations for coupled planes (orbitals) in situations when an attraction is present only in one plane (orbital). We use the

$-U$ Hubbard Hamiltonian as an appropriate simple model, and employ a combination of Quantum Monte Carlo (QMC) and Bogoliubov-de Gennes (BdG) Mean Field Theory. We will focus on a case analogous to that of the PAM, namely when $U = 0$ in one of the layers. We are interested in both how the interlayer hopping affects the s -wave pairing correlations in a layer with $U < 0$, and also whether pairing can be induced by a “proximity effect” in the $U = 0$ layer. Such behavior would be directly analogous to the “RKKY” spin polarization cloud which is induced in the conduction band by the presence of the local moments in the PAM. A particularly interesting issue is whether the QPT which occurs at commensurate filling also occurs in the doped case.

The remainder of this paper is organized as follows: In Sec. II we write down the precise model and give an overview of the QMC and BdG computational methodologies. Secs. III and IV present the BdG and QMC results respectively. Sec. V recaps our conclusions.

II. MODEL AND COMPUTATIONAL METHODS

Our starting point is the two layer (orbital) attractive Hubbard Hamiltonian,

$$\begin{aligned} H = & -t \sum_{\langle ij \rangle l \sigma} (c_{il\sigma}^\dagger c_{jl\sigma} + c_{jl\sigma}^\dagger c_{il\sigma}) \\ & - V \sum_{i\sigma} (c_{i1\sigma}^\dagger c_{i2\sigma} + c_{i2\sigma}^\dagger c_{i1\sigma}) - \sum_{il\sigma} \mu_l c_{il\sigma}^\dagger c_{il\sigma} \\ & - \sum_i |U_1| (n_{i1\uparrow} - \frac{1}{2})(n_{i1\downarrow} - \frac{1}{2}) . \end{aligned} \quad (1)$$

Here an intralayer kinetic energy term $c_{il\sigma}^\dagger c_{jl\sigma}$ describes the creation of a fermion with spin σ on site i of layer l and its destruction on site j of the same layer. A second interlayer kinetic energy term $c_{il\sigma}^\dagger c_{il'\sigma}$ hybridizes the two layers l, l' . Fermions of different spin feel an attractive interaction $-|U_l|$ on layer l . The chemical potentials μ_l control the filling. Our lattice geometry consists of two coupled square lattice of linear size L . We choose $U_1 < 0$ in the ‘superconducting’ plane and $U_2 = 0$ in the metallic one.

At half-filling, a particle-hole transformation formalizes the similarity of the repulsive and attractive models. The vanishing of antiferromagnetic order with increasing V for $U > 0$ bilayers immediately implies that ground state pairing (and charge density wave order, with which it is degenerate) must be destroyed as V grows for $U < 0$. However, whereas AF order occurs only at half-filling (and only at $T = 0$) in the 2D repulsive Hubbard Hamiltonian, superconductivity appears away from half-filling, and at a finite (Kosterlitz-Thouless) transition temperature^{24,25}, in the attractive Hubbard Hamiltonian. This opens up fundamentally new issues in the attractive case. Whether the fermions on sites in adjacent layers will still lock into a local object and destroy long range order when the filling is incommensurate is an interesting question. The absence of a sign problem in the case of the attractive Hubbard model enables the study of low tem-

peratures even when the filling is incommensurate, allowing access to ground state properties.

We perform “determinant” QMC⁹ simulations of the Hamiltonian, Eq. 1 by writing down a path integral for the partition function Z . The exponential of the interaction term U_l is decoupled with a Hubbard-Stratonovich field which allows the trace of the remaining exponentials of quadratic forms of the fermion operators to be performed analytically. The result is a sum over configurations of the Hubbard-Stratonovich field with a weight which takes the form of the product of the determinants of two matrices of dimension the spatial lattice size, one for each spin species. In the case of attractive interaction the two matrices, and hence their determinants, are identical, so that the weight is a perfect square and there is no sign problem.

We present results here for the real space pair correlation functions in the two orbitals,

$$\begin{aligned} P_l(j) &= \langle \Delta_{i+j,l} \Delta_{i,l}^\dagger \rangle \\ \Delta_i^\dagger &= c_{i1\uparrow}^\dagger c_{i1\downarrow}^\dagger \end{aligned} \quad (2)$$

and also their associated structure factors,

$$\mathcal{P}_s^l = \frac{1}{N} \sum_j P_l(j) \quad (3)$$

as a functions of interband hybridization V , on-site attraction U_l , density ρ , and temperature T . The long distance behavior of $P_l(j)$ yields the square of the superconducting order parameter, as does the lattice size dependence of the structure factor.

Eq. 1 can also be studied in Mean Field Theory via the solution of the BdG equations. In this approach, the four fermion (interaction) term is decoupled in the Hamiltonian itself,

$$\begin{aligned} \mathcal{H}_{\text{eff}} = & -t \sum_{\langle ij \rangle l \sigma} (c_{il\sigma}^\dagger c_{jl\sigma} + c_{jl\sigma}^\dagger c_{il\sigma}) \\ & - V \sum_{i\sigma} (c_{i1\sigma}^\dagger c_{i2\sigma} + c_{i2\sigma}^\dagger c_{i1\sigma}) - \sum_{il\sigma} \tilde{\mu}_{il} c_{il\sigma}^\dagger c_{il\sigma} \\ & - \sum_i |U_1| [\Delta_{i1} c_{i1\uparrow}^\dagger c_{i1\downarrow}^\dagger + \Delta_{i1}^* c_{i1\downarrow} c_{i1\uparrow}] . \end{aligned} \quad (4)$$

Here the gap $\Delta_{il} = \langle c_{i1\uparrow} c_{i1\downarrow} \rangle$ and density $\langle n_{il\sigma} \rangle = \langle c_{il\sigma}^\dagger c_{il\sigma} \rangle$ are determined self-consistently by diagonalizing the quadratic BdG Hamiltonian and putting together the eigenvalues and eigenvectors appropriately to compute refined values which are inserted back in the Hamiltonian in an iterative process. A related BdG treatment of superconductivity in the presence of randomness (spatially varying μ_i) is given in [10,11]. $\tilde{\mu}_{il} = \mu + |U_l| \langle n_{il} \rangle / 2$ includes a site-dependent Hartree shift with $\langle n_{il} \rangle = \sum_\sigma \langle n_{il\sigma} \rangle$.

In the general case, when inhomogeneous terms are present in the Hamiltonian, or are expected to develop spontaneously, (like the charge and spin stripes of the doped, repulsive Hubbard model), the order parameter and densities are allowed to depend on site index and the diagonalization must be done numerically. If translation invariance is present, Eq. 4 can be

diagonalized analytically by going to momentum space. The resulting momentum sums are typically still done numerically, but larger lattices can be studied. We have implemented both approaches in the work presented here.

Although inhomogeneous Hartree-Fock theory allows for spatial variation of the densities and superconducting order parameters, the expectation values in Eq. 4 are independent of imaginary time, unlike the fluctuating Hubbard-Stratonovich field in the QMC approach. This leads to a less accurate treatment of interparticle correlations, but a numerically much more simple problem. In particular, larger spatial lattices can be studied, and the BdG solution can exhibit broken symmetry so that Δ itself can be nonzero, rather than having to be extracted from the asymptotics of the correlation function Eq. 2. Here the combination of QMC and BdG will serve to provide complementary information.

In the case of the BdG calculations our focus will be on the value of the order parameter Δ as a function of the same parameters as varied in the QMC. As mentioned above, the asymptotic value of $P_l(j)$ is a measure of Δ^2 . The BdG approach, since it neglects fluctuations, yields larger values of Δ than those of the QMC, which is an exact method.

III. BOGOLIUBOV-DE GENNES RESULTS

The results of BdG calculations are summarized in Fig. 1. We consider two layers with $U_1/t = -8$ and $U_2 = 0$, at a density of $\rho = 0.8$ electrons per site and study the evolution of the pairing correlation, Δ_l , in the two layers as a function inter-layer coupling, V . Pairing in the correlated layer is suppressed by coupling to the non-correlated layer and eventually destroyed completely at a critical V_c , analogous to the destruction of antiferromagnetism by singlet formation in the repulsive case. A further interesting feature of Fig. 1 is that the $l = 2$ layer, with $U_2 = 0$, develops induced pairing with the onset of inter-layer coupling. The pairing amplitude, P_2 , increases with increasing V up to a maximum before decreasing and eventually vanishing at V_c . For $V > V_c$, the ground state consists of weakly interacting inter-layer dimers. Crucially, the pairing order parameter in *both* layers remains non-zero over a finite range of inter-layer coupling – the induced pairing reported previously at half-filling extends to finite dopings. In the next section, we present extensive QMC results to confirm and complement the BdG results.

IV. QUANTUM MONTE CARLO RESULTS

A. Half Filling

We begin our discussion of QMC results at half-filling, $\rho_1 = \rho_2 = 1$. As discussed previously, this corresponds to the particle-hole symmetric point $\mu_1 = \mu_2 = 0$ where there exists an exact mapping to the repulsive Hubbard model and the results can be benchmarked against previous studies of the Hubbard model [7,8]. Lattices of the form $2 \times L \times L$, with $4 \leq L \leq 14$ were studied with periodic boundary conditions

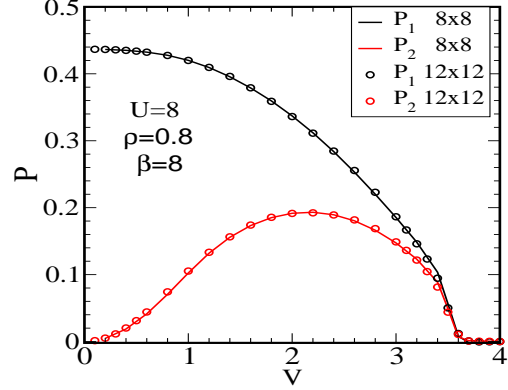


FIG. 1: Bogoliubov-de Gennes result for 8×8 and 12×12 bilayer lattices, $\beta = 8$, $U_1 = -8$, $\rho = 0.8$. The figure shows that there is an induced SC in the noninteracting layer, with negligible finite size effects.

over a wide range of inter-layer hybridization, and on-site interaction for the interacting layer. An inverse temperature $\beta t = L$ was found to be sufficient for the observables to have converged to their ground state values.

The spatial dependence of the pair correlations $P_l(j)$ at half-filling ($\rho = 1$), intersheet hybridization $V = 0.75t$, and interactions $U_1 = -6$, $U_2 = 0$ is shown in Fig. 2. The separation j follows a trajectory along the x axis to maximal x separation $(\frac{L}{2}, 0)$ on a lattice with periodic boundary conditions, and then to $(\frac{L}{2}, \frac{L}{2})$ before returning to separation $(0, 0)$. Results for lattices with $L = 8, 12$ are shown in the figure. The interacting layer $l = 1$ exhibits clear long range order with $P_1(j)$ nearly independent of j beyond a separation of approximately $\frac{L}{4}$. The noninteracting layer $l = 2$ also exhibits proximity-effect induced long range order, although the correlation function is roughly an order of magnitude smaller. This corresponds to an order parameter Δ_l which is approximately a factor of three smaller.

Increasing the inter-layer hybridization reveals that the pair structure factor for the interacting layer, P_s^1 , decreases monotonically and eventually the intra-layer pairing is destroyed at some critical V_c . On the other hand, the pairing structure factor for the non-interacting layer P_s^2 varies non-monotonically with V . It is vanishingly small at small V . As V increases, long-range pairing correlations increase, reach a maximum at an intermediate V (which depends on the strength of on-site interaction in the interacting layer) and then decrease continuously to zero at V_c . For $V > V_c$, the ground state is dominated by *inter*-layer singlets. Fig. 3 shows the finite size dependence of the pairing structure factor for the two layers at several values of V . For $V \gtrsim 1.6$, both P_s^1 and P_s^2 extrapolate to zero in the thermodynamic limit indicating the absence of intra-layer pairing in this regime.

Here and further, the finite size scaling was done by linear fit in the plane $1/L - P_s^l$. The scatter of the data in Fig. 3 for different values of the interlayer hybridization V is dominated

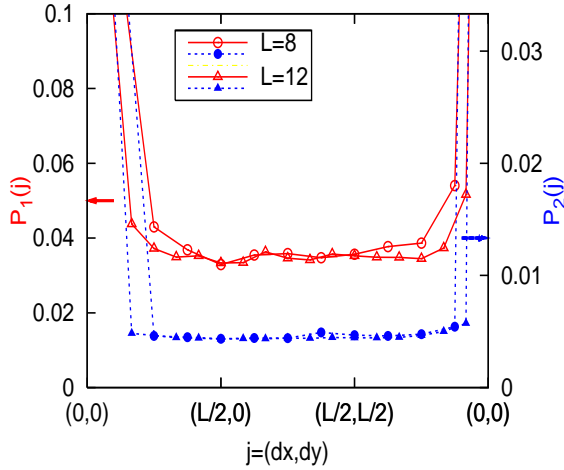


FIG. 2: The dependence of the ground state pair correlation functions, $P_{1,2}(j)$, on separation j in a bilayer system comprised of one correlated layer coupled to an uncorrelated layer for two different lattice sizes L . The system is at half-filling, $\rho = 1$, with interplane hybridization $V = 0.8t$, and on-site interaction strength $U_1 = -6t$ for the correlated layer. The correlation functions converge to non-zero value at large separations, providing clear evidence for long-range order. Despite the absence of interactions, there is proximity-effect induced long-range order in the uncorrelated layer, $l = 2$, with an order parameter Δ_2 approximately a factor of three lower than for the correlated layer. As in Fig. 1, finite size effects are modest.

by the error bars associated with the linear fit to the structure factor on different lattice sizes used in the extrapolation, as opposed to the statistical errors for an individual run. The data scatter serves as a stand-in to provide a visual indication of the uncertainty in the calculation.

B. Incommensurate Filling

We now turn to the case of doped planes. As mentioned in the Introduction, this is interesting for two reasons. First, there is a possibility of a finite temperature KT transition because the CDW-SC symmetry is broken. Second, simulations of coupled, doped repulsive layers at low T are not possible. Hence there is no DQMC information available for the nature of magnetism in coupled layers away from half-filling. Our simulations address this issue, albeit for attractive on-site interactions.

The results in Fig. 4 confirm unambiguously that induced pairing in the uncorrelated layer extends to finite dopings away from half-filling; indeed the pair correlation functions in the two layers are qualitatively similar to those at half-filling. Pairing in the correlated layer decreases monotonically to zero at a finite V_c and that in the non-interacting layer increases rapidly from zero as the inter-layer hybridization is turned on, reaches a maximum value at intermediate V and then decreases to zero. At intermediate to strong values of the on-site interaction ($|U| \gtrsim 6t$), the ground state of a system of coupled correlated and uncorrelated layers away from

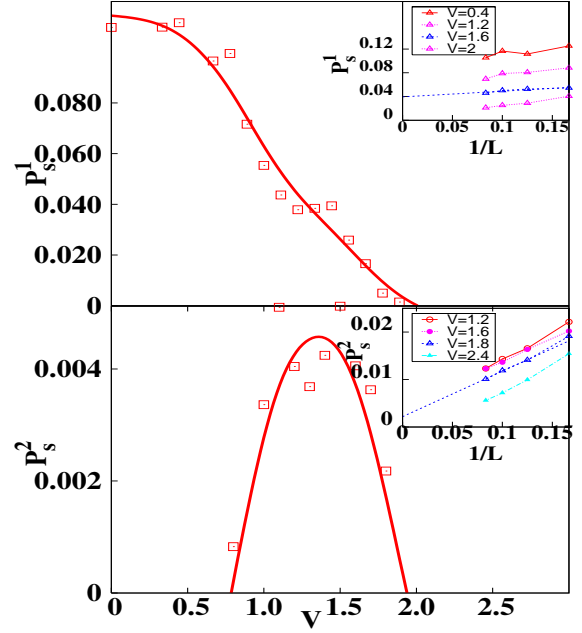


FIG. 3: The pair structure factor for a bilayer at half-filling for attractive on-site interaction in the correlated layer $U = -10t$. The main panels show the extrapolated structure factor as a function of the inter-layer coupling, V . The insets show the extrapolation of the data from finite-sized systems to the thermodynamic limit. Top panel: The pair structure factor in the correlated layer, P_s^1 . For inter-layer hybridization $V \leq 1.6$ the extrapolated structure factor is non-zero indicating the existence of long-range order (LRO). Bottom panel: The pairing structure factor P_s^2 in the non-interacting layer. P_s^2 increases from zero for $V > 0$, signaling the onset of induced pairing. With further increase of V , LRO vanishes simultaneously in both layers.

half-filling consists of intra-layer pair formation in *both* layers over a finite non-zero range of inter-layer coupling. Eventually, at sufficiently strong inter-layer hybridization, pairing in both layers is destroyed and the ground state is dominated by singlet formation between the layers. Induced pairing is found to be absent for $|U| \lesssim 6t$. The simulation results are summarized in Fig. 4 where the extrapolated pairing structure factor for the two layers are shown as a function of the inter-layer hybridization, V , for some representative values of the on-site interaction in the correlated layer at a fixed value of the density, $\rho = 0.8$. The maximum of the pairing structure factor in the uncorrelated layer and the critical value of inter-layer coupling for complete suppression of pairing, V_c , increase with $|U|$. Our results are consistent with the disappearance of pairing in both the layers occurring simultaneously at V_c . The error associated with determining the extrapolated pairing structure factor in the thermodynamic limit limits the accuracy with which V_c can be determined to about $\pm 0.2t$. In a marked departure from the BdG results, the QMC data shows unambiguously that a finite non-zero inter-layer coupling is required for the onset of induced pairing in the uncorrelated layer. This is a consequence of the mean field nature of the

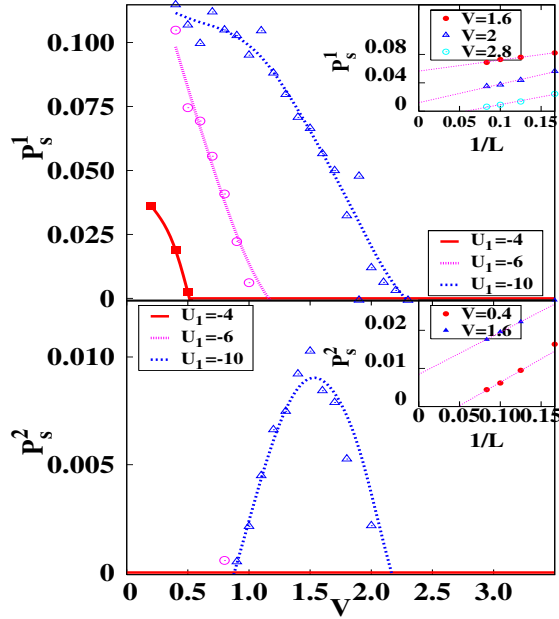


FIG. 4: The pair structure factor for a bilayer away from half-filling, $\rho = 0.8$, for three representative values of the attractive on-site interaction in the correlated layer: $U_1 = -4t, -6t, -10t$. For $|U_1| \lesssim 6t$, $P_s^2 = 0$ at all values of V , indicating the absence of induced pairing. At stronger on-site interaction ($|U_1| > 6t$) in the correlated layer, induced pairing appears in the uncorrelated layer over a finite range of V . The critical V_c for destruction of intra-layer pairing increases with $|U_1|$. Insets: Finite size scaling for $U_1 = -10t$.

BdG results.

Fig. 4 shows that P_1 increases systematically as U changes from $U = -4$ to $U = -10$ and, indeed, shows no sign of saturation. This is at variance with the behavior of the magnetic response of the repulsive Hubbard Hamiltonian which first increases with U but then reaches a maximum at $U \sim 8t$ before falling. This behavior is understood qualitatively from the fact that the superexchange $J = 4t^2/U$ which provides the large U magnetic energy scale declines with U . Thus, for example the Néel temperature of the 3D Hubbard model at half-filling is maximized at $U \sim 8t$. The analog in the attractive Hubbard model is the fact that the pairs become heavy, with an effective hopping $t_{\text{eff}} \sim t^2/U$ associated with the fact that a pair must be (temporarily) broken before it can hop. This analogy suggests the pairing response might also be maximal at an intermediate U . However, because of the sign problem, it is not known from DQMC whether such a non-monotonic behavior exists in the repulsive model away from half-filling. Our results here for the attractive case, which show no sign of saturation with increasing U , suggest that it might not.

Having established the existence of induced pair formation at finite doping and the evolution of the associated structure factor with V , we investigate the dependence of the pairing phenomenon on the density of electrons in the layers. Our results (Fig. 5) show that induced pairing occurs generically at all densities. For all density values studied, the pairing struc-

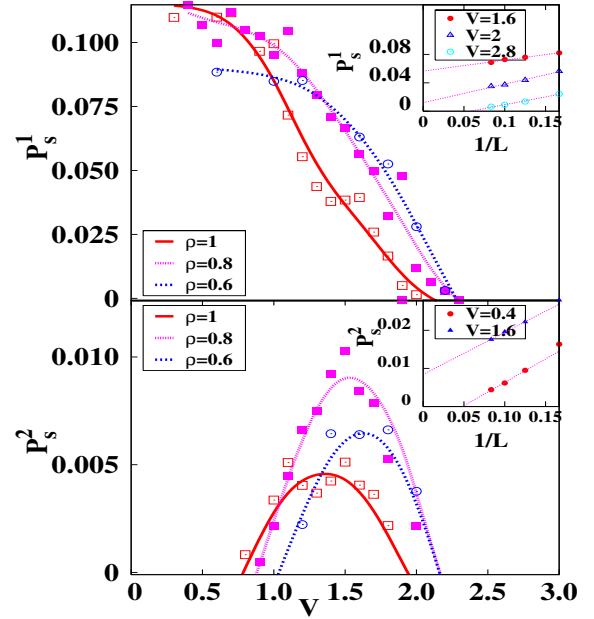


FIG. 5: The pair structure factors at various filling values. Induced pairing occurs at all densities, with the amplitude of induced pairing increasing with doping away from half-filling. Insets: Finite size scaling for $\rho = 0.8$.

ture factor behaves in a qualitatively similar manner, with the pairing strength optimally enhanced at $\rho = 0.8$, as evidenced by the initial increase in peak height with decreasing density. Pairing appears to show a modest decline as the density is reduced further to $\rho = 0.6$, although the effect is rather small given the scatter in the data. Such a non-monotonic doping dependence would be consistent with the behavior of the superconducting T_c with doping for a single 2D sheet. T_c rises abruptly from zero at half-filling where charge density order competes with pairing, but then shows a gradual decline below an optimal doping²⁴.

V. CONCLUSIONS

In this paper we have used Quantum Monte Carlo and Bogoliubov-de Gennes mean field theory to elucidate the properties of a multi-orbital *attractive* Hubbard Hamiltonian. Our key conclusions are the quantification of the induced pairing in a noninteracting orbital by superconductivity in a correlated orbital, and, conversely, the suppression of pairing in an orbital with an attractive interaction through its coupling to a noninteracting orbital.

As we have emphasized in the introduction, analogous issues for repulsive models have a long history. In fact, over the last 4-5 years, the question of ‘orbitally selective Mott transitions’, has been extensively explored. The fundamental objective has been an examination of the density of states to determine whether or not one subsystem can be metallic (zero

energy gap at E_F) and the other insulating (nonzero gap), or whether the coupling forces the transition to occur simultaneously in all orbitals (layers)^{12–23}. Our work suggested that for attractive interactions the destruction of superconductivity at large inter-orbital hybridization V always occurs simultaneously. It is to be noted, however, that it appears that at weak V pairing can exist in the correlated orbital before it is induced in the noninteracting one. That is, we find that for the attractive case at small interlayer coupling, SC exists only in the interacting layer despite the fact that at larger V the vanishing of SC appears at a common V_c .

Our work is related to several other recent determinant QMC and Lanczos studies of the attractive Hubbard model. Assman *et.al*²⁶ found that in an attractive Hubbard model with a smoothly varying chemical potential (such as would be present in a confined ultracold atomic cloud) pairing is significantly increased in the half-filled portion of the lattice through its contact with doped regions. That is, the suppression of superconductivity caused by the appearance of a degenerate

charge density wave phase at $\rho = 1$ is eliminated. Paiva *et.al.* explored a one-dimensional model of borocarbides in which $U < 0$ and $U = 0$ sites alternate²⁷. Superconductivity is found to be possible only above a critical density.

Finally we note that it was recently shown in repulsive models with more than two layers that there can be further interesting and even surprising evolution of magnetic properties with the hopping across an interface between a Mott insulator and a metal²⁸. It would be interesting to pursue related questions in the repulsive model and, in particular whether the formation of a layer of local pairs at the boundary can lead to a shielding of penetration effects.

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